



US011000840B2

(12) **United States Patent**  
**King et al.**

(10) **Patent No.:** **US 11,000,840 B2**  
(45) **Date of Patent:** **\*May 11, 2021**

(54) **THREE-DIMENSIONAL PRINTED OBJECTS FOR CHEMICAL REACTION CONTROL**

*B33Y 50/00* (2014.12); *B33Y 70/00* (2014.12);  
*B33Y 80/00* (2014.12); *B01J 2231/10*  
(2013.01);

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(58) **Field of Classification Search**

CPC ..... *B01J 2231/10*; *B01J 2231/34*; *B01J 2231/4277*; *B01J 31/2295*; *B01J 35/02*;  
*B01J 37/0009*; *B29C 64/10*; *B29C 64/106*;  
*B29C 64/112*; *B29C 64/386*;  
*B33Y 10/00*; *B33Y 50/00*; *B33Y 70/00*;  
*B33Y 80/00*

See application file for complete search history.

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(56) **References Cited**

(\*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

U.S. PATENT DOCUMENTS

3,768,955 A 10/1973 Mc Laughlin  
7,087,109 B2 8/2006 Bredt

(Continued)

This patent is subject to a terminal disclaimer.

FOREIGN PATENT DOCUMENTS

(21) Appl. No.: **16/405,233**

WO 2016038356 A1 3/2016

(22) Filed: **May 7, 2019**

OTHER PUBLICATIONS

(65) **Prior Publication Data**

US 2019/0255518 A1 Aug. 22, 2019

Jakk, "What File Formats are Used in 3D Printing?" www.goprint3D.co.uk, 2 pgs., 2016.

(Continued)

**Related U.S. Application Data**

(63) Continuation of application No. 15/485,726, filed on Apr. 12, 2017, now Pat. No. 10,369,557.

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(51) **Int. Cl.**

*B01J 31/22* (2006.01)

*B33Y 80/00* (2015.01)

(Continued)

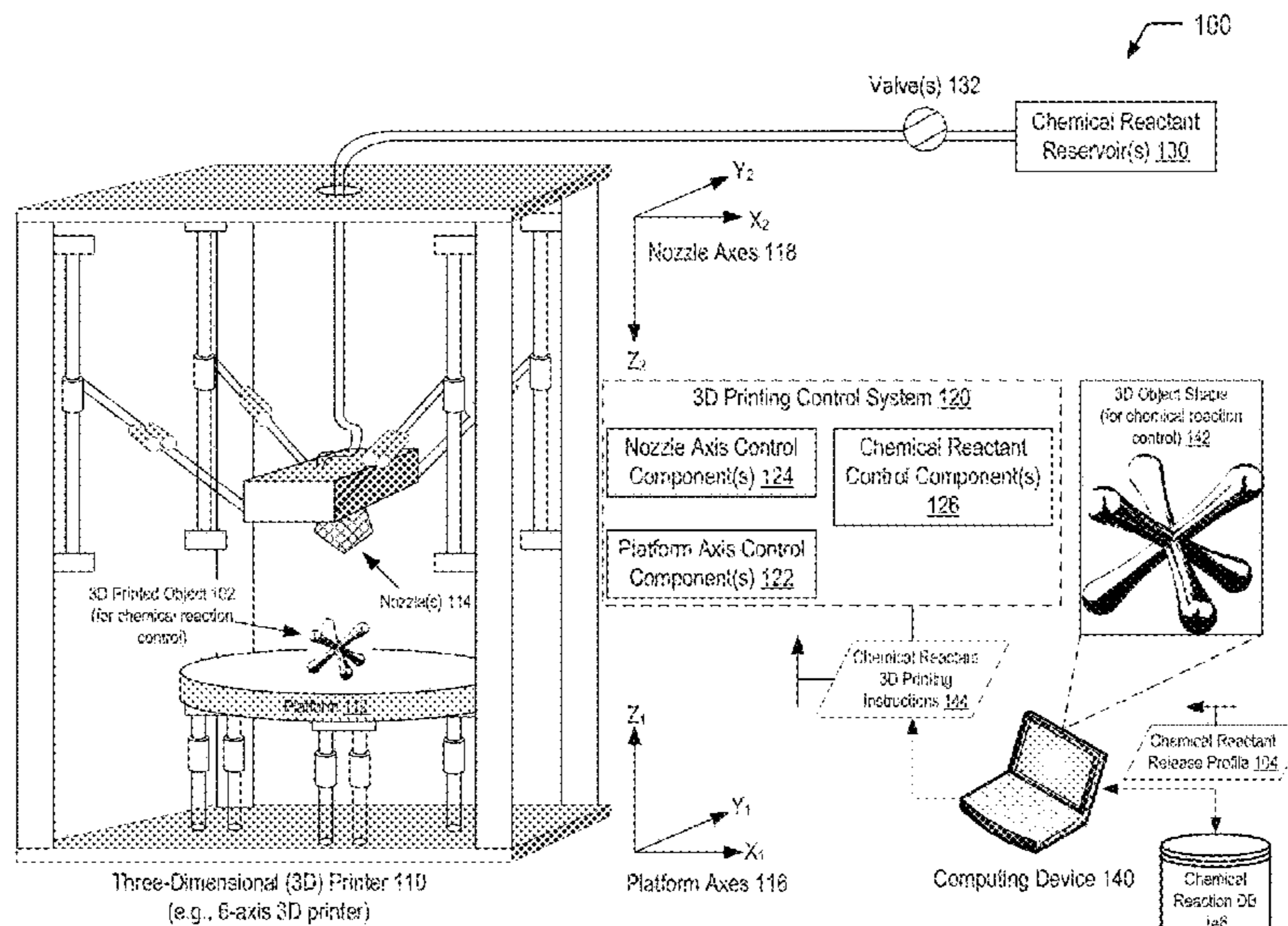
(57) **ABSTRACT**

An article of manufacture includes a three-dimensional (3D) printed object for chemical reaction control. The 3D printed object includes a chemical reactant to be released to control a chemical reaction according to a chemical reactant release profile. The chemical reactant release profile is determined based on a shape of the 3D printed object.

(52) **U.S. Cl.**

CPC ..... *B01J 31/2295* (2013.01); *B01J 35/02* (2013.01); *B01J 37/0009* (2013.01); *B29C 64/10* (2017.08); *B29C 64/106* (2017.08);

**19 Claims, 6 Drawing Sheets**



- (51) **Int. Cl.**  
*B33Y 70/00* (2020.01)  
*B33Y 50/00* (2015.01)  
*B29C 64/10* (2017.01)  
*B29C 64/106* (2017.01)  
*B01J 35/02* (2006.01)  
*B01J 37/00* (2006.01)  
*B33Y 10/00* (2015.01)  
*B29C 64/112* (2017.01)  
*B29C 64/386* (2017.01)
- (52) **U.S. Cl.**  
 CPC .... *B01J 2231/34* (2013.01); *B01J 2231/4277*  
 (2013.01); *B29C 64/112* (2017.08); *B29C*  
*64/386* (2017.08); *B33Y 10/00* (2014.12)
- 2010/0219399 A1 9/2010 Fukushima  
 2012/0177696 A1 7/2012 Wang  
 2013/0337277 A1 12/2013 Dikovsky  
 2014/0329756 A1 11/2014 Nguyen et al.  
 2014/0336808 A1\* 11/2014 Taylor ..... B29C 64/393  
 700/98  
 2016/0067177 A1 3/2016 Adams  
 2016/0137838 A1\* 5/2016 Rolland ..... B29D 11/00009  
 264/401  
 2016/0271878 A1\* 9/2016 Nuechterlein ..... C22C 1/0491  
 2016/0354315 A1 12/2016 Li  
 2017/0001377 A1\* 1/2017 Meisner ..... B29C 64/40  
 2018/0281295 A1\* 10/2018 Tibbits ..... B29C 64/118  
 2018/0297020 A1 10/2018 King  
 2018/0297021 A1 10/2018 King

OTHER PUBLICATIONS

(56) **References Cited**

U.S. PATENT DOCUMENTS

7,261,542 B2 8/2007 Hickerson  
 8,017,055 B2 9/2011 Davidson  
 9,156,205 B2 10/2015 Mark  
 2003/0099708 A1 5/2003 Rowe  
 2006/0208388 A1 9/2006 Bredt  
 2008/0069961 A1\* 3/2008 Sarkar ..... E21B 36/008  
 427/384  
 2008/0220061 A1\* 9/2008 Pryce Lewis ..... A61K 9/2893  
 424/471

Krassenstein, Future Buildings to be 3D Printed Out of Rubber  
 Tires, Salt, Paper & More—Ronald Rael’s REAL 2015 Presenta-  
 tion, 3DPrint.com, The Voice of 3D Printing Technologies (online),  
 Jun. 23, 2015, 9 pages.  
 List of IBM Patents or Patent Applications Treated as Related, May  
 6, 2019, 2 pgs.  
 NUS, NUS Engineering team develops novel technology to “print”  
 customised tablets for personalised medicine, NUS News, National  
 University of Singapore online (NU.edu.sg), May 25, 2016, 2 pages.

\* cited by examiner

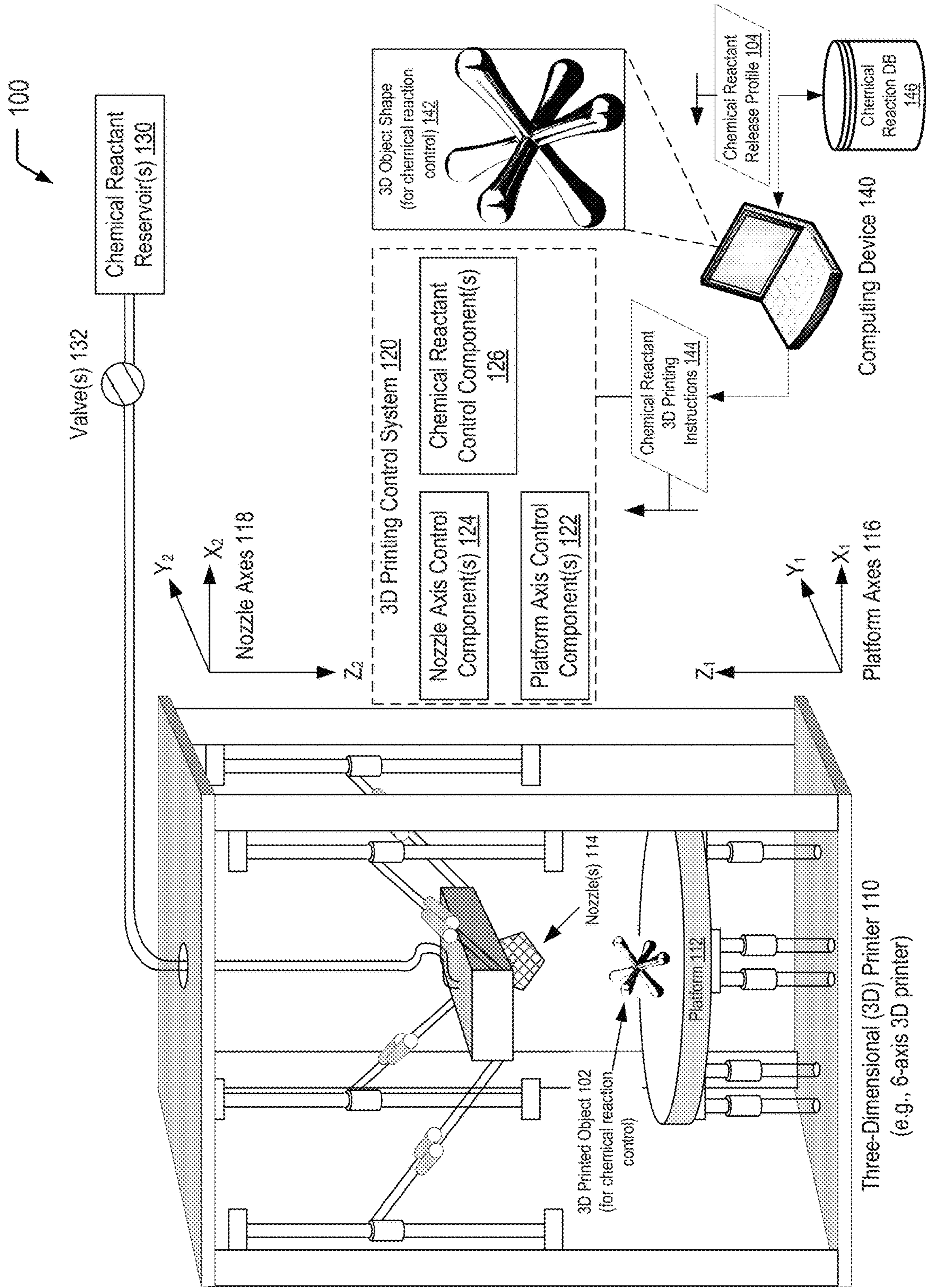


FIG. 1

200

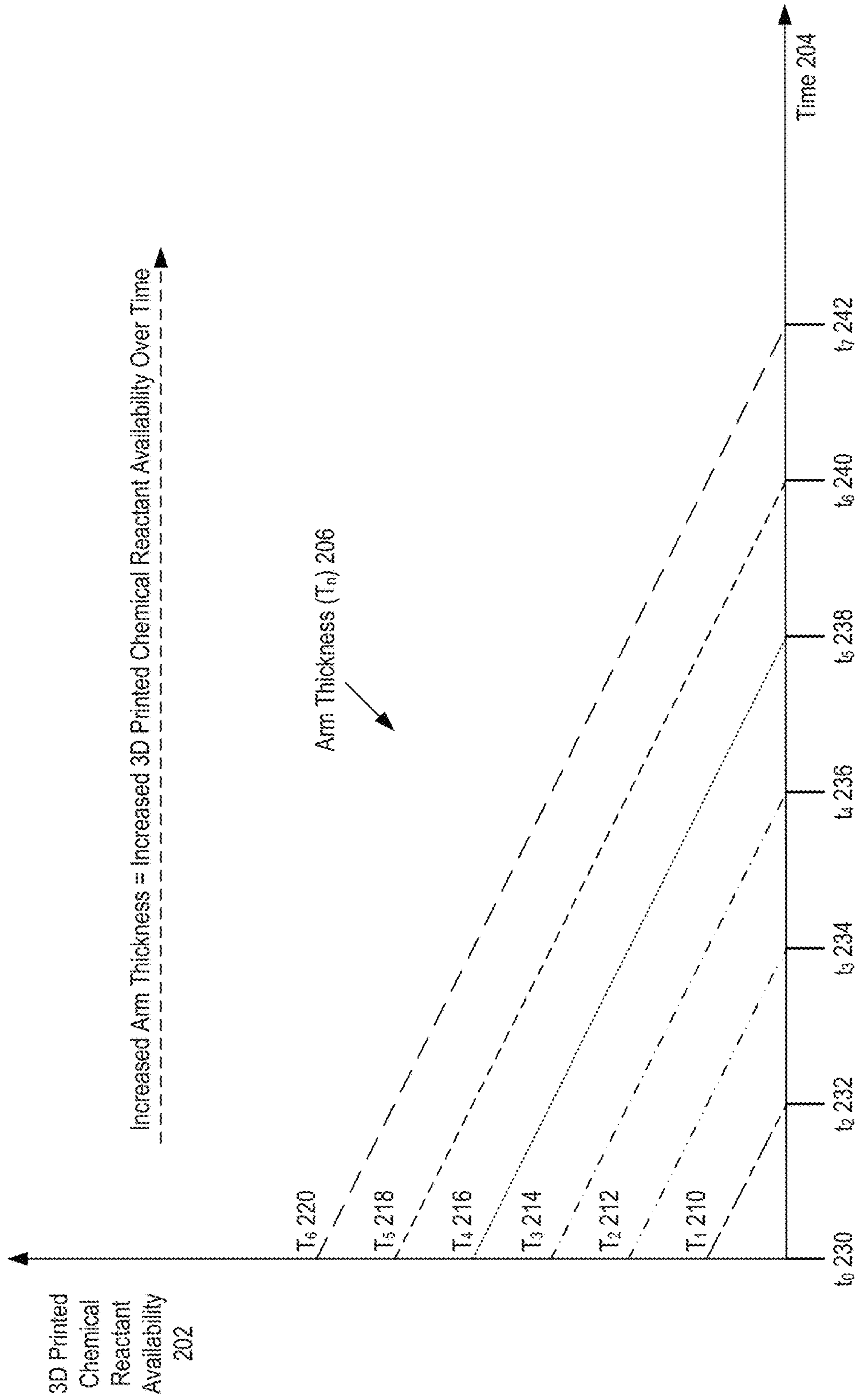


FIG. 2

300

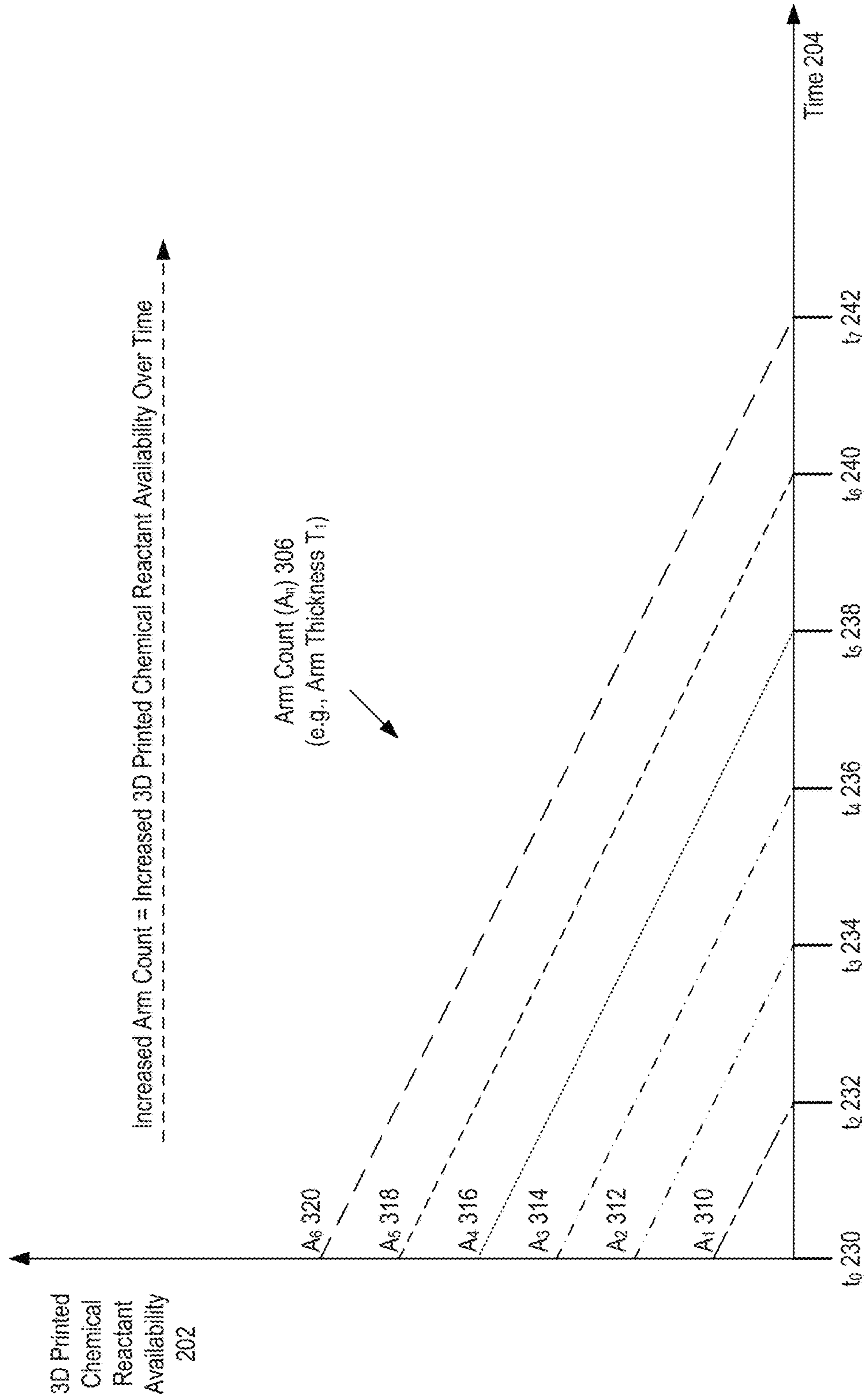


FIG. 3

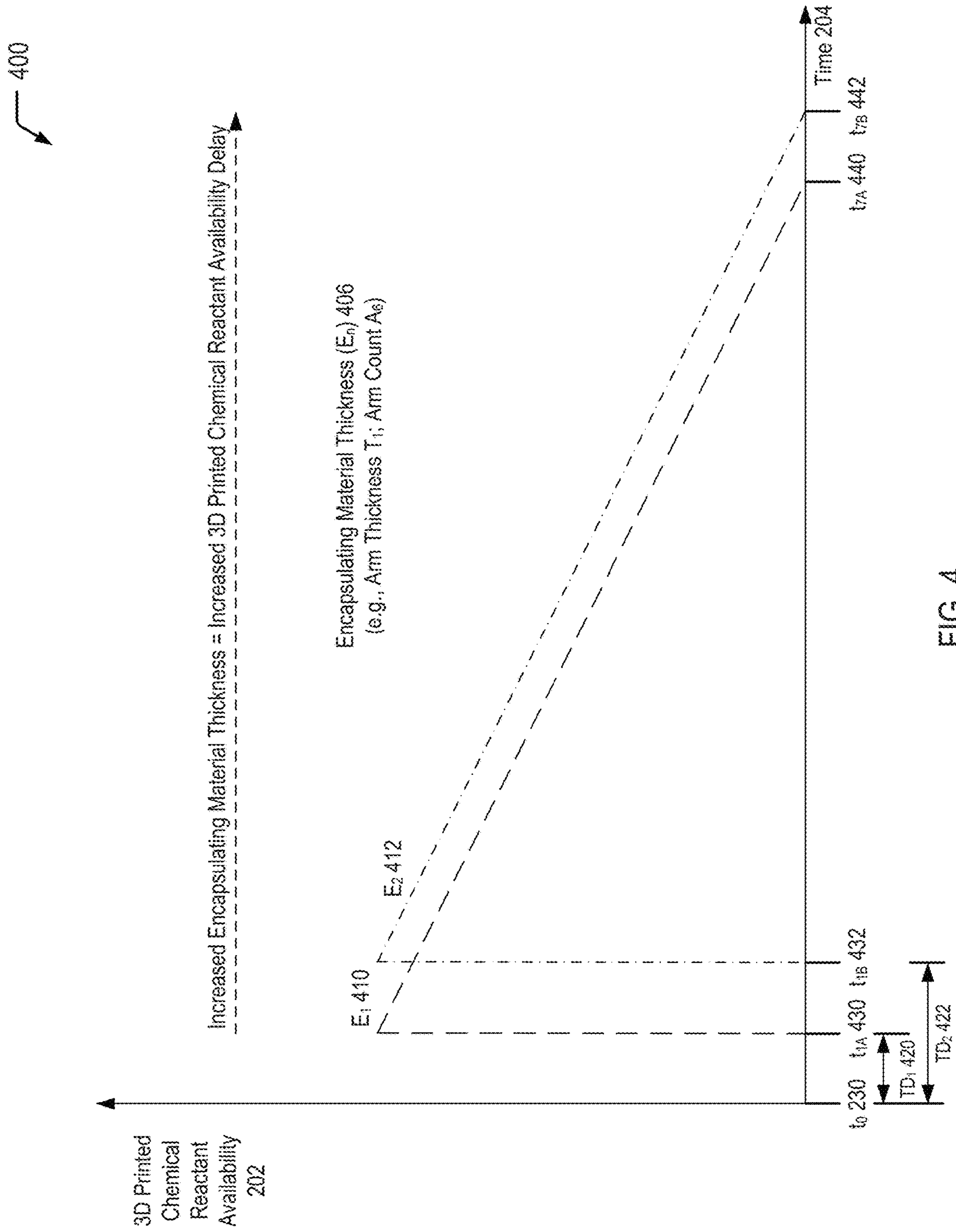


FIG. 4

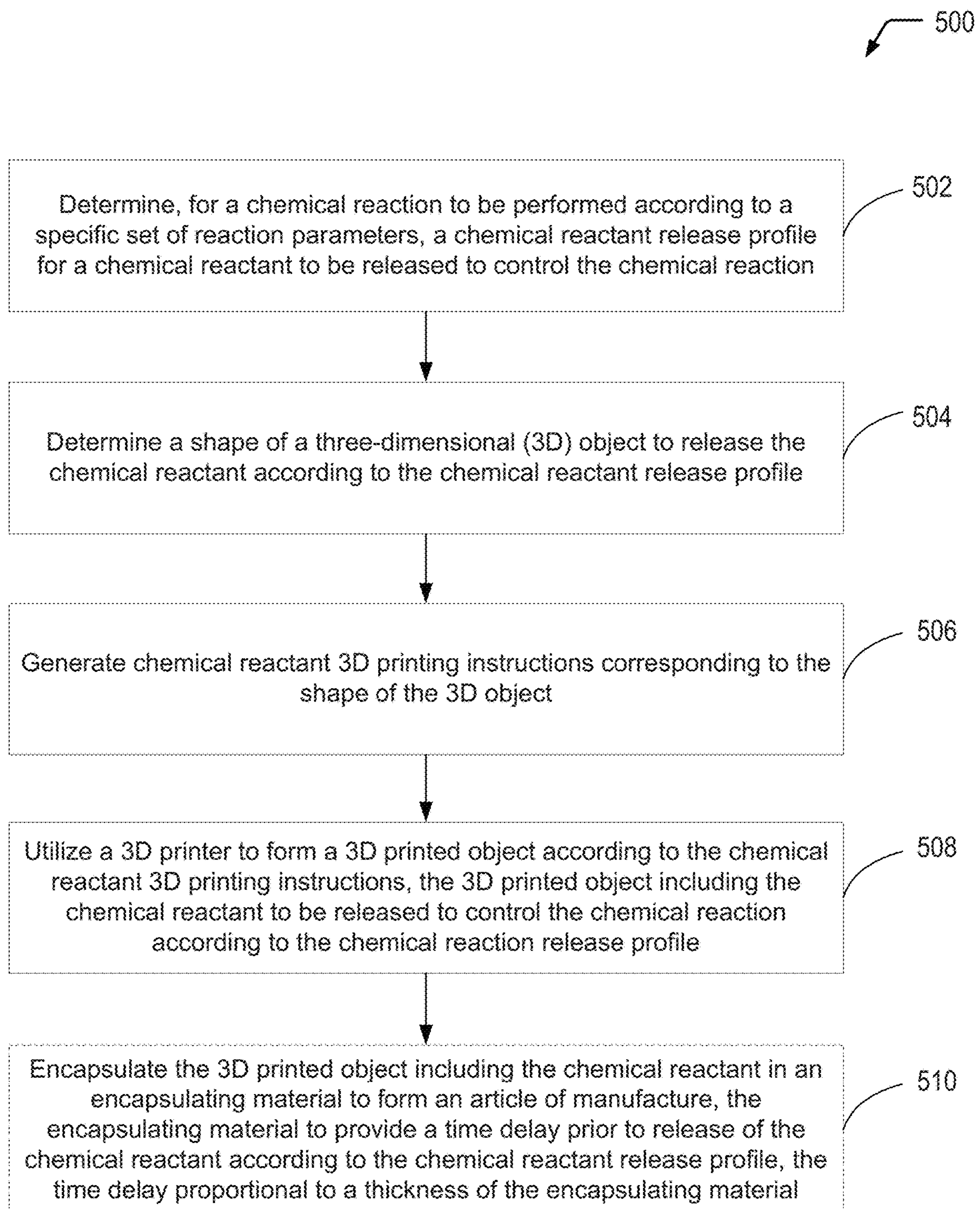


FIG. 5

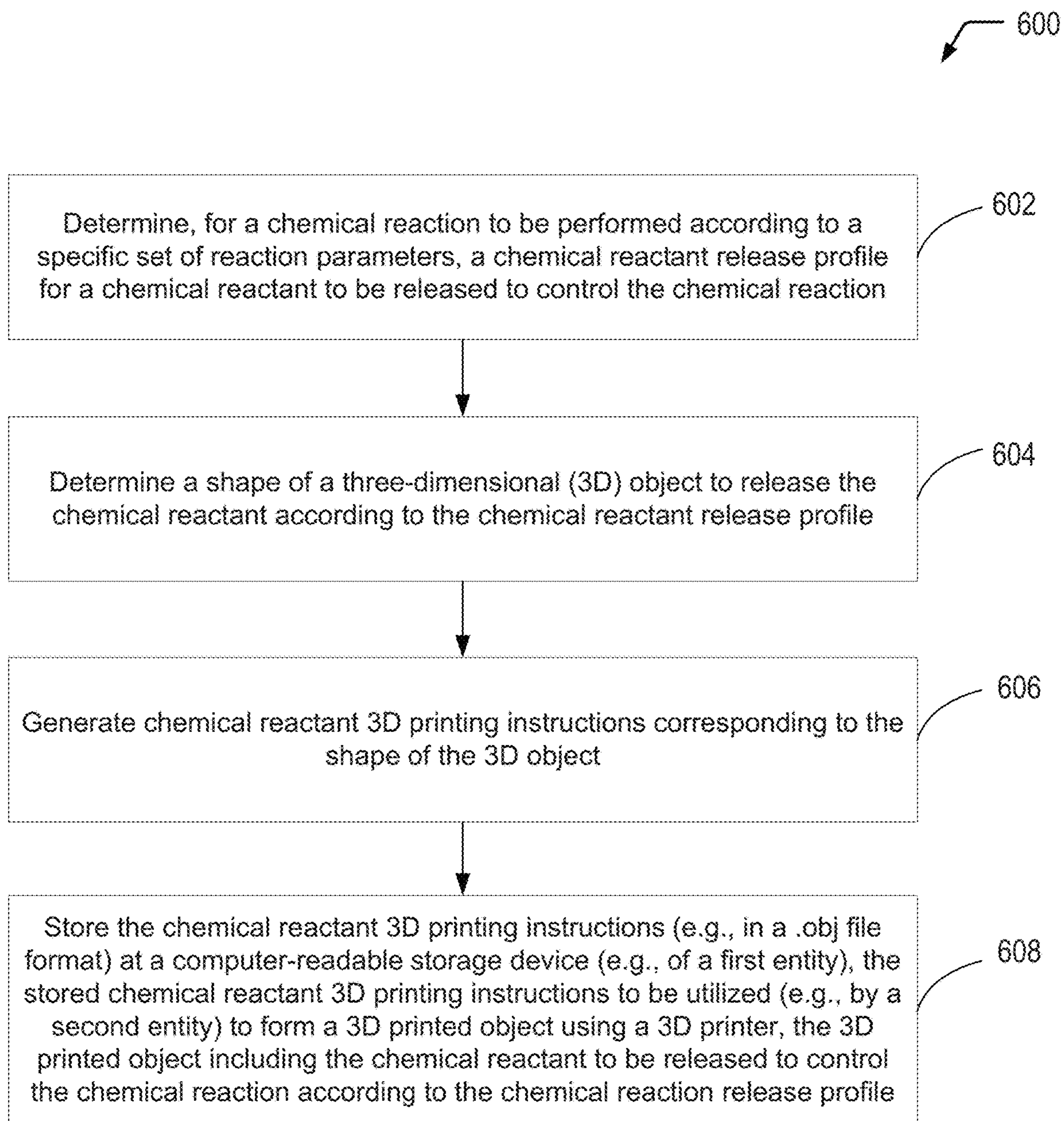


FIG. 6



## 1

THREE-DIMENSIONAL PRINTED OBJECTS  
FOR CHEMICAL REACTION CONTROL

## BACKGROUND

Three-dimensional (3D) printing technology offers exciting possibilities in such varied contexts as rapid prototyping and customized patient-centric drug delivery, among numerous other contexts.

## SUMMARY

According to an embodiment, an article of manufacture is disclosed. The article of manufacture includes a three-dimensional (3D) printed object for chemical reaction control. The 3D printed object includes a chemical reactant to be released to control a chemical reaction according to a chemical reactant release profile. The chemical reactant release profile is determined based on a shape of the 3D printed object.

According to another embodiment, a process of forming a 3D printed object for chemical reaction control is disclosed. The process includes determining, for a chemical reaction to be performed according to a specific set of reaction parameters, a chemical reactant release profile for a chemical reactant to be released to control the chemical reaction. The process includes determining a shape of a 3D object to release the chemical reactant according to the chemical reactant release profile. The process also includes generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object. The process further includes utilizing a 3D printer to form a 3D printed object according to the chemical reactant 3D printing instructions. The 3D printed object includes the chemical reactant to be released to control the chemical reaction according to the chemical reactant release profile.

According to yet another embodiment, a computer-implemented method is disclosed. The computer-implemented method includes determining, for a chemical reaction to be performed according to a specific set of reaction parameters, a chemical reactant release profile for a chemical reactant to be released to control the chemical reaction. The computer-implemented method also includes determining a shape of a 3D object to release the chemical reactant according to the chemical reactant release profile. The computer-implemented method further includes generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object. The chemical reactant 3D printing instructions are to be utilized to generate a 3D printed object that includes the chemical reactant to be released to control the chemical reaction according to the chemical reactant release profile.

The foregoing and other objects, features, and advantages of the invention will be apparent from the following more particular descriptions of exemplary embodiments of the invention as illustrated in the accompanying drawings wherein like reference numbers generally represent like parts of exemplary embodiments of the invention.

## BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 is a diagram of a system for forming an article of manufacture that includes a 3D printed object for chemical reaction control, according to one embodiment.

FIG. 2 is a diagram illustrating an example of the effect of arm thickness of a 3D printed object that includes one or more arms on the availability of a 3D printed chemical reactant over time.

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FIG. 3 is a diagram illustrating an example of the effect of a number of arms of a 3D printed object that includes one or more arms on the availability of a 3D printed chemical reactant over time.

FIG. 4 is a diagram illustrating an example of the effect of a thickness of an encapsulating material surrounding a 3D printed object on the delayed availability of a 3D printed chemical reactant.

FIG. 5 is a flow diagram depicting a particular embodiment of a process of forming a 3D printed object for chemical reaction control.

FIG. 6 is a flow diagram depicting a particular embodiment of a computer-implemented method of generating chemical reactant 3D printing instructions to be utilized to form a 3D printed object for chemical reaction control.

## DETAILED DESCRIPTION

The present disclosure describes three-dimensional (3D) printed objects for chemical reaction control, processes for generating chemical reactant 3D printing instructions, and processes of utilizing a 3D printer to form 3D printed objects for chemical reaction control according to the chemical reactant 3D printing instructions. The 3D printed objects of the present disclosure are also referred to herein as “reaction vessels” to indicate that the 3D printed objects include chemical reactant(s) to be released to control a chemical reaction according to a specific set of reaction parameters.

In the present disclosure, the specific set of reaction parameters are utilized to generate a chemical reaction release profile, and the chemical reaction release profile is utilized to determine an appropriate shape of an object to be 3D printed into a reaction vessel. The chemical reactant(s) are formed into the appropriate shape using a 3D printer, and the resulting 3D printed reaction vessel may be utilized to control a chemical reaction by releasing the chemical reactant(s) in a manner that is consistent with the specific set of reaction parameters. In some cases, the 3D printed reaction vessels of the present disclosure may enable rapid prototyping of various concentration/time-release profiles for reaction control. Additionally, the 3D printed reaction vessels of the present disclosure may enable one entity to efficiently reproduce a chemical reaction according to reaction parameters specified by another entity. To illustrate, in some cases, the 3D printed reaction vessels may be manufactured according to the specific set of reaction parameters determined by a research institution or other laboratory, and the 3D printed reaction vessels may be provided to another research institution or laboratory. In other cases, the chemical reactant 3D printing instructions to be utilized to form the 3D printed reaction vessel may be provided to the other entity (e.g., as an object file for a particular type of 3D printer, such as a 6-axis 3D printer), and the other entity may utilize the chemical reactant 3D printing instructions to form the 3D printed reaction vessel. Thus, the 3D printed objects for chemical reaction control of the present disclosure may enable improved reproducibility of a particular chemical reaction, such as by an entity with less chemical reaction control expertise.

Referring to FIG. 1, a diagram illustrates an example of a system 100 for forming an article of manufacture that includes a 3D printed object 102 for chemical reaction control, according to one embodiment. The 3D printed object 102 includes a chemical reactant (or multiple chemical reactants) to be released to control a chemical reaction that is to be performed according to a specific set of reaction parameters. As described further herein, the specific set of

reaction parameters may be utilized to determine an appropriate shape of the 3D printed object **102** such that the 3D printed object **102** releases the chemical reactant(s) according to a chemical reaction release profile **104** in order to reproduce the chemical reaction according to the specific set of reaction parameters. FIG. **1** depicts an illustrative, non-limiting example in which the shape of the 3D printed object **102** is similar to a toy jack that has multiple arms (e.g., six arms in the example of FIG. **1**). It will be appreciated that the 3D printed object **102** may have an alternative geometric shape (or an alternative thickness or arm count in the case of the toy jack shape) such that the 3D printed object **102** releases the chemical reactant(s) according to a chemical reaction release profile that corresponds to the specific set of reaction conditions. For example, as illustrated and further described herein with respect to FIGS. **2** and **3**, arm thickness and/or arm count values may be adjusted to increase/decrease the availability of a chemical reactant over time. Further, while not shown in the example of FIG. **1**, in some cases, the 3D printed object **102** (or a portion of the 3D printed object **102**, such as a subset of the arms) may be surrounded by an encapsulating material in order to introduce a time delay prior to release of the chemical reactant(s) according to the chemical reactant release profile, as illustrated and further described herein with respect to FIG. **4**.

In the particular embodiment depicted in FIG. **1**, the system **100** includes a 3D printer **110** that includes a platform **112** and a nozzle **114** (or multiple nozzles) that may be independently rotatable about multiple axes. In the particular embodiment depicted in FIG. **1**, the 3D printer **110** is a 6-axis 3D printer that is capable of controlling movement of the platform **112** along three platform axes **116** (identified as axis  $X_1$ , axis  $Y_1$ , and axis  $Z_1$  in FIG. **1**) and movement of the nozzle **114** along three nozzle axes **118** (identified as axis  $X_2$ , axis  $Y_2$ , and axis  $Z_2$  in FIG. **1**). In other embodiments, alternative types of 3D printers may be utilized depending on a complexity of a shape of a particular 3D printed object that is satisfactory to reproduce a particular set of chemical reaction parameters.

The 3D printer **110** is configured to form the 3D printed object **102** for chemical reaction control. In the embodiment depicted in FIG. **1**, the 3D printer **110** includes a 3D printing control system **120** that may include multiple 3D printing control components. In the example of FIG. **1**, the 3D printing control system **120** includes a platform axis control component **122** (or multiple components), a nozzle axis control component **124** (or multiple components), and a chemical reactant control component **126** (or multiple components). The system **100** includes a chemical reactant reservoir **130** (or multiple reservoirs) to store a chemical reactant (or multiple chemical reactants) to be delivered to the nozzle(s) **114** during 3D printing operations responsive to control signals received from the chemical reactant control component(s) **126**.

In the example of FIG. **1**, the system **100** further includes a computing device **140** that may be configured to determine a shape **142** of a 3D object that is satisfactory to release the chemical reactant according to the chemical reactant release profile **104**. The chemical reactant release profile **104** may be determined based on data for a particular chemical reaction that is stored at a chemical reaction database **146**, as described further herein. The computing device **140** may be further configured to generate chemical reactant 3D printing instructions **144** corresponding to the shape **142** of the 3D object. The platform axis control component(s) **122** may be configured to control movement of the platform **112** along the three platform axes **116** according to the chemical

reactant 3D printing instructions **144** received from the computing device **140**. The nozzle axis control component(s) **124** may be configured to control movement of the nozzle(s) **114** along the three nozzle axes **118** according to the chemical reactant 3D printing instructions **144** received from the computing device **140**. The chemical reactant control component(s) **126** may be configured to control release of chemical reactant(s) from the chemical reactant reservoir(s) **130** (e.g., using one or more valves **132** in fluid communication with the nozzle(s) **114**) according to the chemical reactant 3D printing instructions **144** received from the computing device **140**.

The computing device **140** may be configured to determine the shape **142** of the 3D object for a particular set of reaction parameters corresponding to the chemical reactant release profile **104**. In the illustrative, non-limiting example of FIG. **1**, the shape **142** of the 3D object corresponds to a toy jack shape having six arms. It will be appreciated that numerous other alternative shapes may be utilized, with the particular shape selected such that the chemical reactant is released from the 3D printed object **102** in a manner that corresponds to the particular set of reaction parameters. An example of an alternative shape includes a sphere that includes multiple concentric layers (similar to a “jaw-breaker” shape), with each layer including “patches” of a chemical reactant (or multiple chemical reactants). The thickness of a particular layer controls the release of the particular chemical reactant(s) within the particular layer as the individual layers are exposed over time during a chemical reaction. As illustrated and further described herein with respect to FIGS. **2-4**, for the example of the toy jack shape, the computing device **140** may determine a particular combination of arm thickness (see FIG. **2**), arm count (see FIG. **3**), and optionally encapsulating material thickness (see FIG. **4**) that is appropriate for a specific set of reaction parameters.

Illustrative, non-limiting examples of chemical reactions to be evaluated by the computing device **140** to determine the shape **142** of the 3D object include cross-coupling polymerization reactions, living polymerization reactions, substitution nucleophilic ( $S_N2$ ) reactions, or Grignard reactions. Examples of living polymerization reactions include a living anionic polymerization reaction, a living cationic polymerization reaction, a living ring-opening metathesis polymerization reaction, a living free radical polymerization reaction, or a living chain-growth polycondensation reaction.

In some cases, a chemical reaction may utilize a catalyst, and the catalyst may correspond to the chemical reactant to be released to control the chemical reaction according to the chemical reactant release profile **104**. In a particular embodiment, the chemical reaction may correspond to a reaction that utilizes a transition metal (e.g., in the form of an organometallic complex) as a catalyst. Some catalytic transition metals may be utilized in a state that is prone to rapid oxidation, such as a Palladium(0) complex or a Nickel(0) complex. During longer reactions involving such transition metal catalysts, there may be a need for monitoring the reaction and adding additional catalyst (as well as the corresponding ligand) in order to ensure that the reaction progresses. In this case, the chemical reactant release profile **104** may identify that an initial concentration of a catalyst is to be added rapidly and that a suitable level of the catalyst is to be maintained via a slow, controlled release of the catalyst. As an illustrative, non-limiting example, the 3D printed object **102** may be suitable for a Yamamoto cross-coupling polymerization reaction, which is used for direct

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coupling of aryl halides with aryl halides using a bis(cyclooctadiene)nickel(0) compound. Such a polymerization reaction may be performed in a mixture of dimethylformamide (DMF) and toluene, and the bis(cyclooctadiene)nickel(0) compound may be included in the 3D printed object **102** and may be encapsulated using a variety of different polymeric materials, such as polystyrene, poly(methylmethacrylate), poly(vinylacetate), among others.

As another example, the chemical reactant release profile **104** may include information for a chemical reaction in which a slow release of catalyst may be utilized to control molecular weight of polymerization, such as control of chain growth or step growth. As another example, the chemical reactant release profile **104** may include information for a multiple-stage reaction and/or a consecutive reaction. To illustrate, a multiple-stage reaction may include a timed release of a single reactant as a reaction progresses, introduction of other reactant(s) as the reaction progresses, or a combination thereof. To illustrate, for an  $S_N2$  reaction, the chemical reactant release profile **104** may identify that a base is to be released first, creating a nucleophile in the reaction, followed by an electrophile. As a further example, the chemical reactant release profile **104** may include information associated with release of a fouling component. As yet another example, the chemical reactant release profile **140** may include information associated with release of chemical(s) into a living polymerization reaction, such as a living anionic polymerization, a living cationic polymerization, a living ring-opening metathesis polymerization, a living free radical polymerization, or a living chain-growth polycondensation reaction.

As yet another example, the chemical reactant release profile **104** may include information that corresponds to a particular set of chemical reaction parameters associated with a Grignard reaction. In this case, the chemical reactant release profile **104** may correspond to slow formation of a Grignard reagent, where bound magnesium is introduced at a rate that is satisfactory to prevent a run-away reaction. To illustrate, in a Grignard reaction, an alkyl halide or an aryl halide (e.g., hexyl bromide, phenyl bromide, etc.) is added to a suspension of magnesium in diethyl ether or tetrahydrofuran (THF). The halide reacts directly with the surface of the magnesium, but the reaction does not happen immediately in most cases. However, once the halide reacts, the reaction is exothermic, and the heat that is added to the reaction mixture accelerates the reaction. As it typically takes time for the reagents to react, the halide concentration can increase rapidly if the reaction is not carefully monitored, potentially resulting in a run-away reaction with a positive feedback loop of more heat increasing the rate of reaction. Accordingly, the halide may be incorporated into the 3D printed object **102** (e.g., within an inert material, such as an ether or a THF-soluble polymer such as polystyrene) at a varied concentration that would result in a slow, controlled release of the halide. In some cases, magnesium may also be incorporated into the 3D printed object **102**.

Thus, FIG. 1 illustrates an example of a system for forming an article of manufacture that includes a 3D printed object for chemical reaction control. The 3D printed object includes a chemical reactant (or multiple chemical reactants) to be released to control a chemical reaction that is to be performed according to a specific set of reaction parameters. In some cases, the 3D printed object may enable rapid prototyping of various concentration/time-release profiles for reaction control. Additionally, the 3D printed object may enable one entity to efficiently reproduce a chemical reaction according to reaction parameters specified by another entity.

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In other cases, the chemical reactant 3D printing instructions to be utilized to form the 3D printed object may be provided to the other entity, and the other entity may utilize the chemical reactant 3D printing instructions to form the 3D printed object. Thus, the 3D printed object may enable improved reproducibility of a particular chemical reaction, such as by an entity with less chemical reaction control expertise.

FIGS. 2-4 illustrate examples of factors that may be utilized by the computing device **140** of FIG. 1 to determine the shape **142** of the 3D object such that the chemical reactant is released from the 3D printed object **102** for chemical reaction control according to a specific set of reaction parameters defined by the chemical reactant release profile **104**.

Referring to FIG. 2, a diagram **200** illustrates an example of the effect of arm thickness of a 3D printed object that includes one or more arms on the availability of a 3D printed chemical reactant over time. While FIG. 2 is designed to illustrate the dependence of the availability of the 3D printed chemical reactant on arm thickness for the toy jack shape with multiple arms depicted in FIG. 1, it will be appreciated that thickness of a particular feature of an alternatively shaped 3D printed object also affects the availability of the 3D printed chemical reactant over time. Further, FIG. 2 depicts the reduced availability of the 3D printed chemical reactant over time as linear decay for illustrative purposes only.

FIG. 2 is a graph that illustrates a relationship between 3D printed chemical reactant availability **202** over time **204** for multiple arm thickness values ( $T_n$ ) **206**. In the example of FIG. 2, six arm thickness values are depicted, with the arm thickness values increasing along the Y-axis, with a first arm thickness value ( $T_1$ ) **210** representing the smallest arm thickness value depicted in FIG. 2. In order of increasing arm thickness, the other arm thickness values include a second arm thickness value ( $T_2$ ) **212**, a third arm thickness value ( $T_3$ ) **214**, a fourth arm thickness value ( $T_4$ ) **216**, a fifth arm thickness value ( $T_5$ ) **218**, and a sixth arm thickness value ( $T_6$ ) **220**. In order to simplify the explanation of the type of analysis performed by the computing device **140** of FIG. 1 with respect to identification of the shape **142** of the 3D object, the first arm thickness value **210** of FIG. 2 corresponds to a nominal thickness value, and the other arm thickness values **212-220** correspond to integer multiples of the first arm thickness value **210**. That is, the second arm thickness value **212** corresponds to  $2\times$  the first arm thickness value **210**; the third arm thickness value **214** corresponds to  $3\times$  the first arm thickness value **210**; the fourth arm thickness value **216** corresponds to  $4\times$  the first arm thickness value **210**; the fifth arm thickness value **218** corresponds to  $5\times$  the first arm thickness value **210**; and the sixth arm thickness value **220** corresponds to  $6\times$  the first arm thickness value **210**.

FIG. 2 illustrates that the 3D printed chemical reactant availability **202** corresponding to the first arm thickness value **210** decreases over a first period of time defined by an initial time ( $t_0$ ) **230** and a second time ( $t_2$ ) **232**. FIG. 2 further illustrates that the 3D printed chemical reactant availability **202** corresponding to the second arm thickness value **212** decreases over a second period of time defined by the initial time ( $t_0$ ) **230** and a third time ( $t_3$ ) **234**; the third arm thickness value **214** decreases over a third period of time defined by the initial time ( $t_0$ ) **230** and a fourth time ( $t_4$ ) **236**; the fourth arm thickness value **216** decreases over a fourth period of time defined by the initial time ( $t_0$ ) **230** and a fifth time ( $t_5$ ) **238**; the fifth arm thickness value **218** decreases

over a fifth period of time defined by the initial time ( $t_0$ ) **230** and a sixth time ( $t_6$ ) **240**; and the sixth arm thickness value **220** decreases over a sixth period of time defined by the initial time ( $t_0$ ) **230** and a seventh time ( $t_7$ ) **242**. In order to simplify the explanation of the type of analysis performed by the computing device **140** of FIG. **1** with respect to identification of the shape **142** of the 3D object, FIG. **2** illustrates that the first period of time defined by the initial time ( $t_0$ ) **230** and the second time ( $t_2$ ) **232** corresponds to a nominal time value, and the other periods of time correspond to integer multiples of the first period of time.

The initial time ( $t_0$ ) **230** corresponds to a time of arm exposure to a chemical reaction. In the example of FIG. **2**, the initial time ( $t_0$ ) **230** corresponds to time zero. As illustrated and further described herein with respect to FIG. **4**, in cases where an encapsulating material surrounds an arm of the 3D printed object **102** of FIG. **1**, there may be a time delay between a time that the arm of the encapsulated 3D printed object is introduced and a time that the arm is exposed to the chemical reaction. As such, while FIG. **2** illustrates an example in which the initial time ( $t_0$ ) **230** is consistent with immediate exposure of the arm upon introduction of the 3D printed object into a chemical reaction, it will be appreciated that the initial time ( $t_0$ ) **230** may be determined based on the time delay that is proportional to a thickness of the encapsulating material.

Thus, FIG. **2** illustrates that one factor to be utilized by the computing device **140** of FIG. **1** to determine the shape **142** of an arm of the 3D object is a desired period of time for the chemical reactant to be released, as defined by the chemical reactant release profile **104**. As illustrated in the example of FIG. **2**, the thickness of the arm may be selected such that the chemical reactant is released from the 3D printed object **102** over the desired period of time.

Referring to FIG. **3**, a diagram **300** illustrates an example of the effect of an arm count of a 3D printed object that includes one or more arms on the availability of a 3D printed chemical reactant over time. While FIG. **3** is designed to illustrate the dependence of the availability of the 3D printed chemical reactant on arm count for the toy jack shape with multiple arms depicted in FIG. **1**, it will be appreciated that a number of particular features of an alternatively shaped 3D printed chemical reactant also affects the availability of the 3D printed chemical reactant. Further, FIG. **3** depicts the reduced availability of the 3D printed chemical reactant over time as linear decay for illustrative purposes only.

FIG. **3** is a graph that illustrates a relationship between the 3D printed chemical reactant availability **202** over time **204** for multiple arm counts ( $A_n$ ) **306** of a particular arm thickness. For ease of illustration purposes, FIG. **3** illustrates an example in which the particular arm thickness value corresponds to the first arm thickness value  $T_1$  **210** depicted in FIG. **2**. In the example of FIG. **3**, six arm count values are depicted, with the number of arms increasing along the Y-axis, with a first arm count ( $A_1$ ) **310** representing a single arm. In order of increasing number of arms, the other arm count values correspond to two arms ( $A_2$ ) **312**, three arms ( $A_3$ ) **314**, four arms ( $A_4$ ) **316**, five arms ( $A_5$ ) **318**, and six arms ( $A_6$ ) **320**.

FIG. **3** illustrates that the 3D printed chemical reactant availability **302** corresponding to the first arm count value **310** decreases over a first period of time defined by the initial time ( $t_0$ ) **230** and the second time ( $t_2$ ) **232**. FIG. **3** further illustrates that the 3D printed chemical reactant availability **202** corresponding to the second arm count value **312** decreases over a second period of time defined by the initial time ( $t_0$ ) **230** and the third time ( $t_3$ ) **234**; the third arm count

value **314** decreases over a third period of time defined by the initial time ( $t_0$ ) **230** and the fourth time ( $t_4$ ) **236**; the fourth arm count value **316** decreases over a fourth period of time defined by the initial time ( $t_0$ ) **230** and the fifth time ( $t_5$ ) **238**; the fifth arm count value **318** decreases over a fifth period of time defined by the initial time ( $t_0$ ) **230** and the sixth time ( $t_6$ ) **240**; and the sixth arm count value **320** decreases over a sixth period of time defined by the initial time ( $t_0$ ) **230** and the seventh time ( $t_7$ ) **242**. In order to simplify the explanation of the type of analysis performed by the computing device **140** of FIG. **1** with respect to identification of the shape **142** of the 3D object, FIG. **3** illustrates that the first period of time defined by the initial time ( $t_0$ ) **330** and the second time ( $t_2$ ) **332** corresponds to a nominal time value, and the other periods of time correspond to integer multiples of the first period of time.

The initial time ( $t_0$ ) **230** corresponds to a time of arm exposure to a chemical reaction. In the example of FIG. **3**, the initial time ( $t_0$ ) **230** corresponds to time zero. As illustrated and further described herein with respect to FIG. **4**, in cases where an encapsulating material surrounds an arm of the 3D printed object **102** of FIG. **1**, there may be a time delay between a time that the arm of the encapsulated 3D printed object is introduced and a time that the arm is exposed to the chemical reaction. As such, while FIG. **3** illustrates an example in which the initial time ( $t_0$ ) **230** is consistent with immediate exposure of the arm upon introduction of the 3D printed object into a chemical reaction, it will be appreciated that the initial time ( $t_0$ ) **230** may be determined based on the time delay that is proportional to a thickness of the encapsulating material.

Thus, FIG. **3** illustrates that one factor to be utilized by the computing device **140** of FIG. **1** to determine the shape **142** of an arm of the 3D object is a desired period of time for the chemical reactant to be released, as defined by the chemical reactant release profile **104**. As illustrated in the example of FIG. **3**, the number of arms may be selected such that the chemical reactant is released from the 3D printed object **102** over the desired period of time.

Referring to FIG. **4**, a diagram **400** illustrates an example of the effect of a thickness of an encapsulating material surrounding a 3D printed object on the delayed availability of a 3D printed chemical reactant. While FIG. **4** is designed to illustrate the dependence of the delayed availability of the 3D printed chemical reactant on a thickness of an encapsulating material surrounding the toy jack shape with multiple arms depicted in FIG. **1**, it will be appreciated that a thickness of an encapsulating material surrounding an alternatively shaped 3D printed object also affects the delayed availability of the 3D printed chemical reactant. Further, FIG. **4** depicts the reduced availability of the 3D printed chemical reactant over time as linear decay for illustrative purposes only.

FIG. **4** is a graph that illustrates a relationship between the 3D printed chemical reactant availability **202** over time **204** for multiple encapsulating material thickness values ( $E_n$ ) **406**. For ease of illustration purposes, FIG. **4** illustrates an example in which the particular arm thickness value corresponds to the first arm thickness value  $T_1$  **210** depicted in FIG. **2** and the arm count corresponds to the sixth arm count  $A_6$  **320** depicted in FIG. **3**. In the example of FIG. **4**, two encapsulating material thickness values are depicted, with a first encapsulating material thickness value ( $E_1$ ) **410** representing a thickness value that is less than a second encapsulating material thickness value ( $E_2$ ) **412**.

FIG. **4** illustrates that, by encapsulating a 3D printed object having the first thickness value **210** of FIG. **2** and the

sixth arm count  $T_6$  **320** of FIG. **3** (i.e., six arms) that is comparable to the shape **142** depicted in FIG. **1** to be used to form the 3D printed object **102**, a time of initial exposure of the arms of the 3D printed object **102** may be delayed for a period of time that is determined based on a thickness of the encapsulating material. To illustrate, for the first encapsulating material thickness value  $E_1$  **410**, the time of initial release of the chemical reactant may be shifted from the initial time ( $t_0$ ) **230** depicted in FIGS. **2** and **3** in order to introduce a first time delay ( $TD_1$ ) **420**. For the second encapsulating material thickness value ( $E_2$ ) **412**, the time of initial release of the chemical reactant may be shifted from the initial time ( $t_0$ ) **230** depicted in FIGS. **2** and **3** in order to introduce a second time delay ( $TD_2$ ) **422**. In order to simplify the explanation of the type of analysis performed by the computing device **140** of FIG. **1** with respect to identification of the shape **142** of the 3D object, the first encapsulating material thickness value ( $E_1$ ) **410** of FIG. **4** corresponds to a nominal encapsulating material thickness value, and the second encapsulating material thickness value ( $E_2$ ) **412** of FIG. **4** correspond to a  $2\times$  multiple of the first encapsulating material thickness value ( $E_1$ ) **410**.

The introduction of the first time delay ( $TD_1$ ) **420** results in the time of initial release of the chemical reactant being shifted from the second time ( $t_2$ ) **232** depicted in FIGS. **2** and **3** to a first delayed time ( $t_{1A}$ ) **430**. Further, the introduction of the first time delay ( $TD_1$ ) **420** results in a shift of the seventh time ( $t_7$ ) **242** of FIGS. **2** and **3** to a first delayed end time ( $t_{7A}$ ) **440**. The introduction of the second time delay ( $TD_2$ ) **422** results in the time of initial release of the chemical reactant being shifted from the second time ( $t_2$ ) **232** depicted in FIGS. **2** and **3** to a second delayed time ( $t_{1B}$ ) **432**. Further, the introduction of the second time delay ( $TD_2$ ) **422** results in a shift of the seventh time ( $t_7$ ) **242** of FIGS. **2** and **3** to a second delayed end time ( $t_{7A}$ ) **442**.

Thus, FIG. **4** illustrates that an encapsulating material surrounding a 3D printed object may be utilized in order to delay the availability of a 3D printed chemical reactant. FIG. **4** illustrates that the delayed availability of the 3D printed chemical reactant is dependent on a thickness of an encapsulating material. Thus, in some chemical reactions in which a delayed availability of a particular chemical reactant is appropriate, the computing device **140** of FIG. **1** may determine an encapsulating thickness value (for a particular arm thickness/arm count) that is satisfactory to reproduce the desired time delay of chemical reactant release from the 3D printed object **102**.

Referring to FIG. **5**, a flow diagram illustrates a particular embodiment of a process **500** of forming a 3D printed object for chemical reaction control. In the particular embodiment depicted in FIG. **5**, the process **500** further includes forming an article of manufacture by encapsulating the 3D printed object in an encapsulating material.

The process **500** includes determining a chemical reactant release profile for a chemical reactant to be released to control a chemical reaction, at **502**. The chemical reaction is to be performed according to a specific set of reaction parameters. For example, referring to FIG. **1**, the computing device **104** may determine the chemical reactant release profile **104** for a particular chemical reaction based on information stored at the chemical reaction database **146**. As previously described herein, the chemical reaction database **146** may store information associated with multiple types of chemical reactions. As illustrative, non-limiting examples, the chemical reaction may include a cross-coupling polymerization reaction, a substitution nucleophilic ( $S_N2$ ) reaction, a Grignard reaction, a living anionic polymerization reac-

tion, a living cationic polymerization reaction, a living ring-opening metathesis polymerization reaction, a living free radical polymerization reaction, or a living chain-growth polycondensation reaction.

The process **500** includes determining a shape of a 3D object to release the chemical reactant according to the chemical reactant release profile, at **504**. For example, referring to FIG. **1**, the computing device **140** may determine the shape **142** of the 3D object to release the chemical reactant according to the chemical reactant release profile **104**. In the particular embodiment depicted in FIG. **1**, the shape **142** of the 3D object is similar to a toy jack that includes multiple arms (e.g., 6 arms in the example of FIG. **1**). As described further herein with respect to FIG. **2**, different arm thickness values may be associated with different 3D printed chemical reactant availability profiles. Additionally, as described further herein with respect to FIG. **3**, different numbers of arms may be associated with different 3D printed chemical reactant availability profiles. In addition, as further described herein with respect to FIG. **4**, in cases where the 3D printed object **102** is to be surrounded by an encapsulating material, different time delay values may be associated with different encapsulating material thickness values. Accordingly, as described further herein with respect to FIGS. **1-4**, the computing device **140** may utilize multiple factors to determine the shape **142** of the 3D object that is appropriate for the chemical reactant release profile **104** in order to achieve a desired 3D printed chemical reactant availability over time that matches the specific set of reaction parameters associated with a particular chemical reaction.

The process **500** includes generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object, at **506**. For example, referring to FIG. **1**, the computing device **140** may generate the chemical reactant 3D printing instructions **144** corresponding to the shape **142** of the 3D object. In a particular embodiment, the chemical reactant 3D printing instructions **144** may be in an object (.obj) file format that is appropriate for the particular 3D printer **110** to be utilized to form the 3D printed object **102**. In the example of FIG. **1**, the 3D printer **110** corresponds to a 6-axis 3D printer. In this case, the chemical reactant 3D printing instructions **144** may include information to be utilized by the 3D printing control system **120** to control movement of the platform **112** about the three platform axes **116** and to control movement of the nozzle(s) **114** about the three nozzle axes **118** in order to dispense chemical reactant (s) at appropriate locations. Each chemical reaction dispensation location corresponds to a particular combination of a platform axis location defined by an  $X_1$ ,  $Y_1$ , and  $Z_1$  value and a nozzle axis location value defined by an  $X_2$ ,  $Y_2$ , and  $Z_2$  value.

The process **500** includes utilizing a 3D printer to form a 3D printed object according to the chemical reactant 3D printing instructions, at **508**. The 3D printed object includes the chemical reactant to be released to control the chemical reaction according to the chemical reactant release profile. For example, referring to FIG. **1**, the 3D printer **110** may be utilized to form the 3D printed object **102** according to the chemical reactant 3D printing instructions **144** received from the computing device **140**. The 3D printed object **102** includes the chemical reactant (or multiple chemical reactants) dispensed from the chemical reactant reservoir(s) **130** via the nozzle(s) **114**. The chemical reactant is to be released from the 3D printed object **102** to control a particular chemical reaction (having a specific set of reaction param-

eters stored at the chemical reaction database **146**) according to the chemical reactant release profile **104**.

In the particular embodiment depicted in FIG. **5**, the process **500** also includes encapsulating the 3D printed object (including the chemical reactant) in an encapsulating material to form an article of manufacture, at **510**. The encapsulating material provides a time delay prior to release of the chemical reactant according to the chemical reactant release profile, where the time delay is proportional to a thickness of the encapsulating material. For example, while not shown in the example of FIG. **1**, the 3D printer **110** may be utilized to encapsulate the 3D printed object **102** in an encapsulating material. As described further herein, in some cases, the encapsulating material may have a shape that is substantially similar to the shape of the 3D printed object **102** (e.g., an encapsulating layer disposed on a surface of a toy jack shape with six arms, in the example of FIG. **1**). In other cases, the encapsulating material may have a second shape that is different from the shape of the 3D printed object **102** (e.g., a spherical shape, a cubic shape, etc.) that is selected to effect a particular time delay that is appropriate for release of the chemical reactant based on the chemical reactant release profile **104**. As previously described herein with respect to FIG. **4**, increasing the encapsulating material thickness may result in an increase in the 3D printed chemical reactant availability delay.

Thus, FIG. **5** illustrates an example of a process of forming a 3D printed object for chemical reaction control. In some cases, the 3D printed object for chemical reaction control may enable rapid prototyping of various concentration/time-release profiles for reaction control. Further, the 3D printed object for chemical reaction control may enable improved reproducibility of a particular chemical reaction. To illustrate, the 3D printed object for chemical reaction control may enable one entity to efficiently reproduce a chemical reaction according to reaction parameters specified by another entity.

Referring to FIG. **6**, a flow diagram illustrates a particular embodiment of a computer-implemented method **600** of generating chemical reactant 3D printing instructions to be utilized to form a 3D printed object for chemical reaction control.

The computer-implemented method **600** includes determining a chemical reactant release profile for a chemical reactant to be released to control a chemical reaction, at **602**. The chemical reaction is to be performed according to a specific set of reaction parameters. For example, referring to FIG. **1**, the computing device **104** may determine the chemical reactant release profile **104** for a particular chemical reaction based on information stored at the chemical reaction database **146**. As previously described herein, the chemical reaction database **146** may store information associated with multiple types of chemical reactions. As illustrative, non-limiting examples, the chemical reaction may include a cross-coupling polymerization reaction, a substitution nucleophilic ( $S_N2$ ) reaction, a Grignard reaction, a living anionic polymerization reaction, a living cationic polymerization reaction, a living ring-opening metathesis polymerization reaction, a living free radical polymerization reaction, or a living chain-growth polycondensation reaction.

The computer-implemented method **600** includes determining a shape of a 3D object to release the chemical reactant according to the chemical reactant release profile, at **604**. For example, referring to FIG. **1**, the computing device **140** may determine the shape **142** of the 3D object to release the chemical reactant according to the chemical reactant

release profile **104**. In the particular embodiment depicted in FIG. **1**, the shape **142** of the 3D object is similar to a toy jack that includes multiple arms (e.g., 6 arms in the example of FIG. **1**). As described further herein with respect to FIG. **2**, different arm thickness values may correspond to different 3D printed chemical reactant availability over time. Additionally, as described further herein with respect to FIG. **3**, different numbers of arms may correspond to different 3D printed chemical reactant availability over time. In addition, as further described herein with respect to FIG. **4**, in cases where the 3D printed object **102** is to be surrounded by an encapsulating material, different time delay values may be associated with different encapsulating material thickness values. Accordingly, as described further herein with respect to FIGS. **1-4**, the computing device **140** may utilize multiple factors to determine the shape **142** of the 3D object that is appropriate for the chemical reactant release profile **104** in order to achieve a desired 3D printed chemical reactant availability over time that matches the specific set of reaction parameters associated with a particular chemical reaction.

The computer-implemented method **600** includes generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object, at **606**. For example, referring to FIG. **1**, the computing device **140** may generate the chemical reactant 3D printing instructions **144** corresponding to the shape **142** of the 3D object.

In the particular embodiment depicted in FIG. **6**, the computer-implemented method **600** also includes storing the chemical reactant 3D printing instructions at a computer-readable storage device, at **608**. The stored chemical reactant 3D printing instructions are to be utilized to form a 3D printed object using a 3D printer. The 3D printed object includes the chemical reactant to be released to control the chemical reaction according to the chemical reaction release profile. For example, referring to FIG. **1**, the computing device **140** may be associated with a first entity, such as a chemist that has developed a particular set of chemical reaction parameters for a chemical reaction. In some cases, it may be desirable for the chemical reaction to be reproducible by a second entity. In this case, after generating the chemical reactant 3D printing instructions **144**, the computing device **140** may store the chemical reactant 3D printing instructions **144** at a computer-readable storage device (not shown in FIG. **1**). The stored chemical reactant 3D printing instructions **144** may be sent to the second entity from the first entity or otherwise made accessible to the second entity (e.g., via a network). In some cases, the stored chemical reactant 3D printing instructions **144** may represent an open-source 3D printing instruction file that may enable efficient validation/reproduction of the chemical reaction by the second entity. In other cases, the stored chemical reactant 3D printing instructions **144** may be proprietary to the first entity.

In a particular embodiment, the computing device **140** (e.g., of a first entity) may store the chemical reactant 3D printing instructions **144** in an object (.obj) file format that is appropriate for the particular 3D printer **110** to be utilized to form the 3D printed object **102**. In the example of FIG. **1**, the 3D printer **110** corresponds to a 6-axis 3D printer that may be associated with a second entity (in some cases). In this case, the stored chemical reactant 3D printing instructions **144** may include information to be utilized by the 3D printing control system **120** to control movement of the platform **112** about the three platform axes **116** and to control movement of the nozzle(s) **114** about the three nozzle axes **118** in order to dispense chemical reactant(s) at

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appropriate locations. Each chemical reaction dispensation location corresponds to a particular combination of a platform axis location defined by an  $X_1$ ,  $Y_1$ , and  $Z_1$  value and a nozzle axis location value defined by an  $X_2$ ,  $Y_2$ , and  $Z_2$  value.

Thus, FIG. 6 illustrates an example of a process of a computer-implemented method of generating chemical reactant 3D printing instructions to be utilized to form a 3D printed object for chemical reaction control. In some cases, the 3D printing instructions may enable one entity to manufacture a 3D printed object for chemical reaction control in order to efficiently reproduce a chemical reaction according to reaction parameters specified by another entity.

It will be understood from the foregoing description that modifications and changes may be made in various embodiments of the present invention without departing from its true spirit. The descriptions in this specification are for purposes of illustration only and are not to be construed in a limiting sense. The scope of the present invention is limited only by the language of the following claims.

What is claimed is:

1. A process of forming a three-dimensional (3D) printed object for chemical reaction control, the process comprising:

determining, by a processor, for a chemical reaction to be performed according to a set of reaction parameters, a chemical reactant release profile for one or more chemical reactants to be released to control the chemical reaction, wherein the chemical reactant release profile indicates a concentration level of each of the one or more chemical reactants;

determining a shape of a three-dimensional (3D) object to release the one or more chemical reactants according to the chemical reactant release profile; and

forming the 3D object in the determined shape, the 3D object formed with a 3D printable fluid that includes at least one of the one or more chemical reactants to be released to control the chemical reaction according to the chemical reactant release profile, and wherein the determined shape includes at least two arms, with a first arm formed with the 3D printable fluid with a first chemical reactant and a second arm formed with the 3D printable fluid with a second chemical reactant.

2. The process of claim 1, wherein the chemical reaction includes a cross-coupling polymerization reaction, a substitution nucleophilic ( $S_N2$ ) reaction, a Grignard reaction, a living anionic polymerization reaction, a living cationic polymerization reaction, a living ring-opening metathesis polymerization reaction, a living free radical polymerization reaction, or a living chain-growth polycondensation reaction.

3. The process of claim 1, further comprising utilizing a 3D printer to encapsulate the 3D object in an encapsulating material.

4. The process of claim 1, further comprising generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object.

5. The process of claim 4, further comprising utilizing a 3D printer to form the 3D object according to the chemical reactant 3D printing instructions.

6. A computer-implemented method comprising:  
determining, by a processor, for a chemical reaction to be performed according to a set of reaction parameters, a chemical reactant release profile for one or more chemical reactants to be released to control the chemical reaction;

determining a shape of a three-dimensional (3D) object to release the one or more chemical reactants according to

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the chemical reactant release profile, wherein the shape of the 3D object includes one or more arms, each of the one or more arms incorporated with at least one of the one or more chemical reactants; and

forming the 3D object according to the shape, the 3D object formed with a 3D printable fluid that includes at least one of the one or more chemical reactants to be released to control the chemical reaction according to the chemical reactant release profile.

7. The computer-implemented method of claim 6, further comprising generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object.

8. The computer-implemented method of claim 7, further comprising utilizing a 3D printer to form the 3D object according to the chemical reactant 3D printing instructions.

9. The computer-implemented method of claim 8, wherein the 3D printer includes a 6-axis 3D printer.

10. The computer-implemented method of claim 9, further comprising storing the chemical reactant 3D printing instructions at a computer-readable storage device of a first entity, the stored chemical reactant 3D printing instructions to be utilized by a second entity to form the 3D object using a 3D printer.

11. The computer-implemented method of claim 10, wherein the first entity performs the chemical reaction according to the set of reaction parameters, and wherein the stored chemical reactant 3D printing instructions are utilized by the second entity to reproduce the chemical reaction according to the set of reaction parameters.

12. The computer-implemented method of claim 10, wherein the chemical reactant 3D printing instructions are stored at the computer-readable storage device in an object (.obj) file format.

13. A system comprising:

a memory; and

a processor in communication with the memory, the processor being configured to perform operations comprising:

determining for a chemical reaction to be performed according to a set of reaction parameters, a chemical reactant release profile for one or more chemical reactants to be released to control the chemical reaction;

determining a shape of a three-dimensional (3D) object to release the one or more chemical reactants according to the chemical reactant release profile, wherein the shape of the 3D object includes one or more arms, each of the one or more arms incorporated with at least one of the one or more chemical reactants; and

forming the 3D object according to the shape, the 3D object formed with a 3D printable fluid that includes at least one of the one or more chemical reactants to be released to control the chemical reaction according to the chemical reactant release profile.

14. The system of claim 13, wherein the operations further comprise:

generating chemical reactant 3D printing instructions corresponding to the shape of the 3D object.

15. The system of claim 14, wherein the operations further comprise:

utilizing a 3D printer to form the 3D object according to the chemical reactant 3D printing instructions.

16. The system of claim 15, wherein the 3D printer includes a 6-axis 3D printer.

17. The system of claim 16, wherein the operations further comprise:

storing the chemical reactant 3D printing instructions at a computer-readable storage device of a first entity, the

stored chemical reactant 3D printing instructions to be utilized by a second entity to form the 3D object using the 3D printer.

**18.** The system of claim **17**, wherein the first entity performs the chemical reaction according to the set of reaction parameters, and wherein the stored chemical reactant 3D printing instructions are utilized by the second entity to reproduce the chemical reaction according to the set of reaction parameters.

**19.** The system of claim **17**, wherein the chemical reactant 3D printing instructions are stored at the computer-readable storage device in an object (.obj) file format.

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